

High-energy asymptotics of the spectrum of a periodic square-lattice quantum graph

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Abstract. We investigate a periodic quantum graph in form of a square lattice with a general self-adjoint coupling at the vertices. We analyze the spectrum, in particular, its high-energy behaviour. Depending on the coupling type, bands and gaps have different asymptotics. Bands may be flat even if the edges are coupled, and non-flat band widths may behave like $\mathcal{O}(n^j)$, $j = 1, 0, -1, -2, -3$, as the band index $n \rightarrow \infty$. The gaps may be of asymptotically constant width or linearly growing with the latter case being generic.

1. Introduction

Origins of the quantum graph concept can be traced back to Linus Pauling's considerations about the structure of organic molecules in 1930's, however, it was roughly the last two decades when the subject became very popular and its true richness has been revealed. The reason for that was not only the fact that quantum graphs represent a suitable model of numerous systems prepared by solid state physicists. Equally important was the inherent structure of such models which allowed us to study effects uncommon in the "usual" quantum mechanics coming from the nontrivial topological structure of graph structures as well as from the fact that they mix features corresponding to different dimensionalities. The bibliography concerning quantum graphs is nowadays extensive indeed and we restrict ourselves to quoting the proceedings volume of a recent topical programme at Isaac Newton Institute and references therein [AGA08].

One often studied class are periodic graphs. Their spectrum has predictably a band structure, however, in distinction to the usual Schrödinger operators they can exhibit

under particular geometric conditions also infinitely degenerate eigenvalues manifesting invalidity of the unique continuation principle [Ku05]. The aim of the present paper is to investigate the spectrum in a particular example of periodic graphs, namely two-dimensional square lattices with a general self-adjoint coupling at the vertices. This generalizes earlier work in which lattices with δ and δ'_s couplings were studied [Ex96, EG96].

A motivation for the present extension comes from different sources. First of all, the general vertex coupling became more interesting after several recent results — cf. [KZ01, EP09, CET10] and references therein — showing how it can be approximated by graphs or network systems with suitably scaled potentials illustrating thus that it is not just a mathematical object but also something which can be, in an approximative sense at least, realized physically. Secondly, already the mentioned examples of δ and δ'_s couplings demonstrated that different couplings yield different asymptotical behaviour of spectral bands and gaps at high energies.

These asymptotics can have interesting dynamical consequences. Recall that in the one-dimensional analogue of the present problem, in the generalized Kronig-Penney model, there are three types of asymptotic behaviour [EG99, CS04] and that the one corresponding to the δ' interaction for which spectral gaps are dominating exhibit absence of transport in the Wannier-Stark situation when an electric field is applied [AEL94, Ex95, MS95, ADE98]; we stress that the solution of the Wannier-Stark problem in the other two cases mentioned is still an open question. With these facts in mind it is natural to ask how many types of asymptotic behaviour a two dimensional square lattice can show and what they look like. Our approach to this problem is based on the use of the so-called ST -form of boundary condition introduced in [CET10]. This will allow us to express the band and gap widths by rather simple expressions involving the coupling parameters, from which it is easy to determine how the spectral behaviour is governed by the particular boundary conditions.

We will show that the high-energy behaviour has more types than in the one-dimensional situation. In fact, the problem has sixteen parameters and offers a zoology of solutions. The scope of this issue does not allow us to present a complete classification but we will list all the “generic” cases with respect to the rank of the matrix B in the condition (1) below and single out cases of particular interest. The two-dimensional character of the problem has two main consequences. The first one is a possible occurrence of flat bands, or infinitely degenerate eigenvalues; this is connected with the invalidity of the principle of unique continuation on graphs of nontrivial topology mentioned above. The second remarkable feature is the existence of couplings for which the spectral bands are shrinking as n^{-1} , n^{-2} , or n^{-3} with respect to the band index n . This effect again has no analogue in the one-dimensional situation. The most “generic” situation, however, is the one known from [Ex96, EG96] when the bands are asymptotically of constant widths and gaps are linearly growing.

2. Preliminaries and main result

2.1. Square lattice with a general vertex coupling

As we have said we will consider a square lattice graph. To be concrete, the vertices of Γ are $\{(ma, na) : m, n \in \mathbb{Z}\}$ for a fixed $a > 0$ and the edges are segments of length a connecting points differing by one in one of the two indices. The state Hilbert space is the orthogonal sum of the L^2 spaces on the edges and the Hamiltonian acts as $-\frac{d^2}{dx^2}$ on each of them, with the domain consisting of the corresponding $W^{2,2}$ functions.

It is well known that in order to get a self-adjoint operator one has to impose boundary conditions at graph vertices which couple the vectors $\Psi(0)$ and $\Psi'(0)$ of the boundary values — we choose the variables at all the adjacent edges so that they start at the vertex. The standard form of these conditions is

$$A\Psi(0) + B\Psi'(0) = 0, \quad (1)$$

where A, B are matrices such that $(A|B)$ has maximum rank and AB^* is self-adjoint [KS99]. Being interested in the periodic situation we naturally assume that the matrices A, B are the same at each vertex of the lattice. A drawback of the conditions (1) is that the matrix pair is not unique. There are various ways to mend this problem. One is to rewrite (1) in the form

$$(U - I)\Psi(0) + i(U + I)\Psi'(0) = 0, \quad (2)$$

where U is a unitary matrix. In the quantum graph context these conditions have been proposed in [Ha00, KS00], however, they were known earlier in the general theory of boundary forms [GG91]. It is clear that a distinguished role is played by subspaces of the boundary space values referring to eigenvalues ∓ 1 of U . An alternative way [Ku04] to write the conditions is by means of the corresponding orthogonal projection P and its complement $Q := I - P$: there is a self-adjoint operator L in $Q\mathbb{C}^n$ such that

$$P\Psi(0) = 0, \quad Q\Psi'(0) + LQ\Psi(0) = 0. \quad (3)$$

Here we are going to use yet another version introduced in [CET10] as the *ST-form*,

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi'(0) = \begin{pmatrix} S & 0 \\ -T^* & I^{(n-m)} \end{pmatrix} \Psi(0) \quad (4)$$

using matrices $T \in \mathbb{C}^{m, n-m}$ and a self-adjoint $S \in \mathbb{C}^{m, m}$, where n is the dimension of the boundary value space (which will be four in our case) and $m = n - \dim P \in \{0, \dots, n\}$.

2.2. The main result

Let $H_{S,T}$ is the quantum graph Hamiltonian described above. Our results about its spectrum can be summarized as follows:

Theorem 2.1. (a) *The spectrum of $H_{S,T}$ consists of absolutely continuous spectral bands and infinitely degenerate eigenvalues. Its negative part consists of at most four bands.*

(b) *The high-energy asymptotic behaviour of spectral bands and gaps as a function of the band index n includes the following classes:*

- *flat bands, i.e. infinitely degenerate point spectrum,*
- *bands behaving like $\mathcal{O}(n^j)$, $j = 1, 0, -1, -2, -3$, as $n \rightarrow \infty$,*
- *gaps behaving like $\mathcal{O}(n^j)$, $j = 1, 0$, as $n \rightarrow \infty$.*

Depending on the vertex coupling (1) the high-energy asymptotics of the spectrum may be a combination of the above listed types.

The rest of the paper is devoted to demonstrating of these claims. We will do that by analyzing spectrum of the fiber operator coming from the Bloch-Floquet analysis, discussing subsequently situations corresponding to different values of rank m of the matrix B in the boundary conditions (1). While this procedure serves best our aim, it is not very illustrative from the point of view of particular type of edge coupling. Apart from the trivial case $m = 0$ when the lattice decomposes into separate edges with Dirichlet conditions, each of the other values of m cover several subcases with very different couplings and spectral behaviours. They would deserve a separate discussion which we cannot present here due to volume restrictions and we postpone it to another publication; we limit ourselves to several general statements:

- The generic situation corresponds to $m = 4$ with all the edges coupled and spectral gaps growing linearly with the band index,
- each case $m = 1, 2, 3, 4$ covers a situations with flat bands corresponding to lattice decoupling into separated edges, or pairs of edges,
- the lattice can separate into “one-dimensional” subsets describing generalized Kronig-Penney models on lines or zigzag curves, or to “combs”,
- from the spectral point of view the case $m = 3$ is the richest, including situations with a powerlike shrinking of spectral bands that occurs for the graph decomposed into “combs”.

3. Bloch-Floquet analysis

Since our graph is a -periodic w.r.t. shifts in both directions, we are able to employ the Bloch-Floquet decomposition. The elementary cell is depicted in Fig. 1, together with the notation of the wave function components on the edges.

The analysis follows the same pattern as in [Ex96, EG96] but the general vertex coupling makes it substantially more complicated. The fiber operator corresponding to fixed values of Floquet parameters (quasimomentum components) has a purely discrete spectrum and the number of its negative eigenvalues is at most four. The last claim follows from general principles [We80, Sec. 8.3] and from a comparison to the square

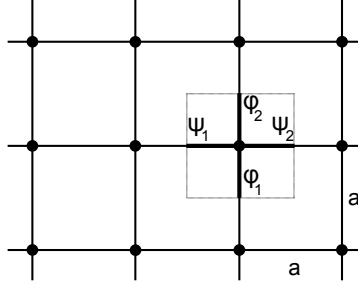


Figure 1. A periodic two-dimensional network

graph Hamiltonian with Kirchhoff coupling at the vertices the spectrum of which equals by [Ex96] \mathbb{R}^+ ; it is enough to notice that the Floquet component of this operator and that of a general $H_{S,T}$ have a common symmetric restriction with deficiency indices (n, n) , $n \leq 4$. Note also that the bands may overlap in general; an example can be constructed using boundary conditions which separate motion in the two directions leading to two families of generalized Kronig-Penney models.

Our main interest concerns the positive part of the spectrum, and as usual we are thus going to investigate solutions of the corresponding stationary Schrödinger equation with energy $E = k^2$, $k > 0$. It is obvious that they are at each edge linear combinations of the functions e^{ikx} and e^{-ikx} , specifically

$$\begin{aligned} \psi_1(x) &= C_1^+ e^{ikx} + C_1^- e^{-ikx}, & x \in [-a/2, 0] \\ \psi_2(x) &= C_2^+ e^{ikx} + C_2^- e^{-ikx}, & x \in [0, a/2] \\ \varphi_1(x) &= D_1^+ e^{ikx} + D_1^- e^{-ikx}, & x \in [-a/2, 0] \\ \varphi_2(x) &= D_2^+ e^{ikx} + D_2^- e^{-ikx}, & x \in [0, a/2] \end{aligned} \tag{5}$$

By assumption, they have to satisfy the boundary conditions at the vertex, i.e. it holds

$$A \begin{pmatrix} \psi_1(0) \\ \psi_2(0) \\ \varphi_1(0) \\ \varphi_2(0) \end{pmatrix} + B \begin{pmatrix} -\psi_1'(0) \\ \psi_2'(0) \\ -\varphi_1'(0) \\ \varphi_2'(0) \end{pmatrix} = 0. \tag{6}$$

In addition to that, of course, they have to satisfy Bloch-Floquet conditions,

$$\begin{aligned} \psi_2(a/2) &= e^{i\theta_1} \psi_1(-a/2) & \varphi_2(a/2) &= e^{i\theta_2} \varphi_1(-a/2), \\ \psi_2'(a/2) &= e^{i\theta_1} \psi_1'(-a/2) & \varphi_2'(a/2) &= e^{i\theta_2} \varphi_1'(-a/2), \end{aligned} \tag{7}$$

for fixed values of the quasimomentum components $\theta_1, \theta_2 \in (-\pi, \pi]$. Substituting (5) into (7) allows us to express the variables C_2^\pm and D_2^\pm in terms of C_1^\pm and D_1^\pm ,

$$C_2^\pm = C_1^\pm \cdot e^{i(\theta_1 \mp ak)}, \quad D_2^\pm = D_1^\pm \cdot e^{i(\theta_2 \mp ak)}. \tag{8}$$

Using these relations we eliminate C_2^\pm and D_2^\pm from (5), after that we substitute (5) into (6). Simple manipulations then yield the following condition,

$$[(AM + ikBN)D] \begin{pmatrix} C_1^+ \\ C_1^- \\ D_1^+ \\ D_1^- \end{pmatrix} = 0, \quad (9)$$

where $D := \text{diag} \left(e^{\frac{i}{2}(\theta_1 - ak)}, e^{\frac{i}{2}(\theta_1 + ak)}, e^{\frac{i}{2}(\theta_2 - ak)}, e^{\frac{i}{2}(\theta_2 + ak)} \right)$ and the matrices M, N are given by

$$M := \begin{pmatrix} e^{-\frac{i}{2}(\theta_1 - ak)} & e^{-\frac{i}{2}(\theta_1 + ak)} & 0 & 0 \\ e^{\frac{i}{2}(\theta_1 - ak)} & e^{\frac{i}{2}(\theta_1 + ak)} & 0 & 0 \\ 0 & 0 & e^{-\frac{i}{2}(\theta_2 - ak)} & e^{-\frac{i}{2}(\theta_2 + ak)} \\ 0 & 0 & e^{\frac{i}{2}(\theta_2 - ak)} & e^{\frac{i}{2}(\theta_2 + ak)} \end{pmatrix},$$

$$N := \begin{pmatrix} -e^{-\frac{i}{2}(\theta_1 - ak)} & e^{-\frac{i}{2}(\theta_1 + ak)} & 0 & 0 \\ e^{\frac{i}{2}(\theta_1 - ak)} & -e^{\frac{i}{2}(\theta_1 + ak)} & 0 & 0 \\ 0 & 0 & -e^{-\frac{i}{2}(\theta_2 - ak)} & e^{-\frac{i}{2}(\theta_2 + ak)} \\ 0 & 0 & e^{\frac{i}{2}(\theta_2 - ak)} & -e^{\frac{i}{2}(\theta_2 + ak)} \end{pmatrix}.$$

It follows from (8) that the functions (5) correspond to a nonzero solution *iff* $(C_1^+, C_1^-, D_1^+, D_1^-)$ is a nonzero vector. Consequently, a number k^2 belongs to the spectrum of the Hamiltonian if and only if (9) has a non-trivial solution for some pair (θ_1, θ_2) , in other words, if there are θ_1, θ_2 such that $\det[(AM + ikBN)D] = 0$ which can be simplified to

$$\det(AM + ikBN) = 0. \quad (10)$$

Our aim is to analyze the spectral asymptotics in dependence on the coupling type. Since four edges join at each vertex, the problem has 16 real parameters. We will take them into account through the *ST* form (4) of the boundary conditions, i.e. we set

$$-A = \begin{pmatrix} S & 0 \\ -T^* & I^{(4-m)} \end{pmatrix}, \quad B = \begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix},$$

where $m := \text{rank}(B)$. Obviously, each value of m has to be discussed separately.

4. The case of $m = 0$, or Dirichlet decoupled edges

Consider first the simplest situation when $B = 0$, $A = -I$. The *ST*-form of boundary conditions is then obviously invariant with respect to the edge labelling and the spectral condition (10) acquires the form $\det(-M) = 0$. Since $\det(-M) = \det(M) = -4 \sin^2 ak$, this requires $\sin ak = 0$, hence the spectrum consists of infinitely degenerate eigenvalues,

$$\sigma(H) = \left\{ \left(\frac{n\pi}{a} \right)^2 \mid n \in \mathbb{N} \right\}.$$

5. The case of $m = 1$

The admissible couplings form a seven-parameter family corresponding to the choice

$$B = \begin{pmatrix} 1 & t_1 & t_2 & t_3 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A = - \begin{pmatrix} s & 0 & 0 & 0 \\ -\overline{t_1} & 1 & 0 & 0 \\ -\overline{t_2} & 0 & 1 & 0 \\ -\overline{t_3} & 0 & 0 & 1 \end{pmatrix}$$

with $s \in \mathbb{R}$ and $t_j \in \mathbb{C}$. Note that while in general the boundary conditions in the ST -form are not invariant with respect to the edge renumbering, we can choose without loss of generality the “privileged one” corresponding to the first component. A direct calculation of the determinant in (10) leads to the spectral condition

$$-4k \sin ak \left[(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak - 2\Re(t_1 e^{i\theta_1} + \overline{t_2} t_3 e^{i\theta_2}) \right] - 4s \sin^2 ak = 0.$$

We see that the condition is solved again by $\frac{n\pi}{a}$ for $n \in \mathbb{N}$. In addition to that, there are solutions coming from the equation

$$(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak - 2\Re(t_1 e^{i\theta_1} + \overline{t_2} t_3 e^{i\theta_2}) = -\frac{1}{k} s \sin ak. \quad (11)$$

Recall that $k^2 > 0$ is in the spectrum if there are $\theta_1, \theta_2 \in (-\pi, \pi]$ which together with k satisfy (11). It is convenient to rewrite the range of the expression $\Re(t_1 e^{i\theta_1} + \overline{t_2} t_3 e^{i\theta_2})$ using a single parameter as follows:

Observation 5.1. *It holds*

$$\{ \Re(t_1 e^{i\theta_1} + \overline{t_2} t_3 e^{i\theta_2}) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} = \{ (|t_1| + |t_2| \cdot |t_3|) \cos \vartheta \mid \vartheta \in (-\pi, \pi] \}.$$

The spectral condition (11) then yields the following requirement:

$$(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak - 2(|t_1| + |t_2| \cdot |t_3|) \cos \vartheta = -\frac{1}{k} s \sin ak. \quad (12)$$

This conditions has various types of solutions in dependence on the parameter values. Before discussing them, let us mention another useful fact.

Observation 5.2. *It holds $2(|t_1| + |t_2| \cdot |t_3|) \leq 1 + |t_1|^2 + |t_2|^2 + |t_3|^2$ and the equality occurs if and only if $|t_1| = 1 \wedge |t_2| = |t_3|$.*

5.1. Point spectrum

If the expression $|t_1| + |t_2| \cdot |t_3|$ vanishes, i.e. if $t_1 = 0$ and $t_2 = 0 \vee t_3 = 0$ (we may suppose without loss of generality that $t_3 = 0$), then (11) becomes

$$\cotg ak = -\frac{1}{k} \frac{s}{1 + |t_2|^2}. \quad (13)$$

The *rhs* being $\mathcal{O}(k^{-1})$ as $k \rightarrow \infty$ the solutions are obviously close to the numbers $(-\frac{1}{2} + n)\frac{\pi}{a}$ at high energies. Writing them as

$$k = \left(-\frac{1}{2} + n\right) \frac{\pi}{a} + \delta;$$

we get $\cotg ak = a\delta + \mathcal{O}(\delta^3)$ and $\frac{1}{k} = \frac{a}{n\pi} + \mathcal{O}(n^{-2})$. A substitution into (13) and a few manipulations give $\delta = \frac{1}{n\pi} \cdot \frac{-s}{1+|t_2|^2} + \mathcal{O}(n^{-2})$, hence this solution represents the spectral points $k^2 = k_n^2$ behaving like

$$k^2 = \left[\left(-\frac{1}{2} + n\right) \frac{\pi}{a} \right]^2 + \frac{2}{a} \cdot \frac{-s}{1+|t_2|^2} + \mathcal{O}(n^{-1})$$

for $n \rightarrow \infty$. These solutions are independent of the quasimomentum and give rise to flat spectral bands; it is not difficult to see that the corresponding eigenfunctions can be chosen compactly supported.

Let us remark that the boundary conditions studied above mean that the Hamiltonian decouples into a countable direct sum of operators supported on two edges of the graph, or on individual edges if $T = 0$ and $s = 0$, and therefore it is not surprising that the spectrum is pure point.

5.2. Linearly growing spectral bands and gaps

If $|t_1| + |t_2| \cdot |t_3| \neq 0$, we can divide by it and express thus $\cos \vartheta$ from (12). This yields the spectral condition in the form

$$\left| \frac{1 + |t_1|^2 + |t_2|^2 + |t_3|^2}{2(|t_1| + |t_2| \cdot |t_3|)} \cos ak + \frac{1}{k} \cdot \frac{s}{2(|t_1| + |t_2| \cdot |t_3|)} \sin ak \right| \leq 1. \quad (14)$$

By Observation 5.2, the coefficient of $\cos ak$ at the *lhs* cannot be smaller than one.

In the rest of this section, we focus on the case $|t_1| \neq 1 \vee |t_2| \neq |t_3|$; the remaining situation will be treated in Section 5.3. Since the coefficient of $\sin ak$ is $\mathcal{O}(k^{-1})$, it is evident that (14) can be asymptotically satisfied only away from the points where $|\cos ak| = 1$, in other words, the spectral bands are neighbourhoods of the points $\left[(-\frac{1}{2} + n)\frac{\pi}{a}\right]^2$. Let us set $k = (-\frac{1}{2} + n)\frac{\pi}{a} + d$ and find the range of d . We see that $\cos ak = \sin ad$ and $\frac{1}{k}$ of the n -th band solution is $\mathcal{O}(n^{-1})$, thus (14) can be rewritten as

$$|\sin ad| \leq \frac{2(|t_1| + |t_2| \cdot |t_3|)}{1 + |t_1|^2 + |t_2|^2 + |t_3|^2} + \mathcal{O}(n^{-1}).$$

Hence $ad \leq \Delta := \arcsin \frac{2(|t_1| + |t_2| \cdot |t_3|)}{1 + |t_1|^2 + |t_2|^2 + |t_3|^2}$; note that $\Delta \in (0, \frac{\pi}{2})$ in view of the assumption and Observation 5.2. Then the spectral bands behave like

$$\left(\left[\left(-\frac{1}{2} + n\right) \frac{\pi}{a} - \frac{\Delta}{a} + \mathcal{O}\left(\frac{1}{n}\right) \right]^2, \left[\left(-\frac{1}{2} + n\right) \frac{\pi}{a} + \frac{\Delta}{a} + \mathcal{O}(n^{-1}) \right]^2 \right),$$

which can be rewritten as

$$\left(\left(-\frac{1}{2} + n \right)^2 \frac{\pi^2}{a^2} - 2 \frac{n\pi}{a^2} \Delta + \mathcal{O}(1), \left(-\frac{1}{2} + n \right)^2 \frac{\pi^2}{a^2} + 2 \frac{n\pi}{a^2} \Delta + \mathcal{O}(1) \right)$$

in the high-energy limit, $n \rightarrow \infty$. In other words, both bands and gaps are asymptotically linearly growing with the band index.

5.3. Asymptotically constant spectral gaps

If $|t_1| = 1$ and $|t_2| = |t_3| \neq 0$, the spectral condition (14) has to be treated differently being now of the form

$$\left| \cos ak + \frac{1}{k} \cdot \frac{s}{2(1+|t_2|^2)} \sin ak \right| \leq 1. \quad (15)$$

Let us suppose that $s \neq 0$ — the case $s = 0$ is special and will be discussed below in Section 5.4. Since $|\cos ak| \leq 1$ and the coefficient at $\sin ak$ is small in modulus for large values of k , we see that the condition (15) is violated only in a small one-sided neighbourhood of the points where $|\cos ak| = 1$. To describe the corresponding *gaps*, we set $k = \frac{n\pi}{a} + \delta$, then we have

$$\begin{aligned} \cos ak &= (-1)^n \cdot \left(1 - \frac{(a\delta)^2}{2} + \mathcal{O}(\delta^4) \right), \\ \sin ak &= (-1)^n \cdot a\delta + \mathcal{O}(\delta^3), \\ \frac{1}{k} &= \frac{a}{n\pi} + \mathcal{O}\left(\frac{\delta}{n^2}\right). \end{aligned}$$

Substituting from here into the *negated* condition (15) we obtain the gap condition,

$$\left| 1 - \frac{(a\delta)^2}{2} + \frac{a^2}{n\pi} \frac{s}{2(1+|t_2|^2)} \delta + \mathcal{O}(\delta^4) + \mathcal{O}\left(\frac{\delta^3}{n}\right) + \mathcal{O}\left(\frac{\delta^2}{n^2}\right) \right| > 1,$$

which is, in dependence of the sign of s , solved by

$$\delta \in \begin{cases} \left(\mathcal{O}\left(\frac{1}{n^2}\right), \frac{1}{n\pi} \cdot \frac{s}{1+|t_2|^2} + \mathcal{O}(n^{-2}) \right) & \text{for } s > 0, \\ \left(\frac{1}{n\pi} \cdot \frac{s}{1+|t_2|^2} + \mathcal{O}\left(\frac{1}{n^2}\right), \mathcal{O}(n^{-2}) \right) & \text{for } s < 0. \end{cases}$$

Consequently, the gap boundaries are

$$\left(\frac{n\pi}{a} \right)^2 + \mathcal{O}(n^{-1}) \quad \text{and} \quad \left(\frac{n\pi}{a} \right)^2 + \frac{2}{a} \cdot \frac{s}{1+|t_2|^2} + \mathcal{O}(n^{-1}),$$

in other words, the gap widths are asymptotically constant and spectral bands grow linearly w.r.t. the band number n . Note that this case includes lattices with a *nontrivial* δ coupling discussed in [Ex96, EG96].

5.4. No gaps, spectrum on the nonnegative halfline

It remains to discuss the case with $|t_1| = 1$, $|t_2| = |t_3| \neq 0$ and $s = 0$, when the spectral condition (15) simplifies to $|\cos ak| \leq 1$ which is obviously satisfied for all $k > 0$. Moreover, one checks directly that $0 \in \sigma(H)$, and putting $k = i\kappa$ we find $\sigma(H) \cap (-\infty, 0) = \emptyset$, hence $\sigma(H) = [0, +\infty)$. Referring again to [Ex96, EG96] we note that this includes the case of a lattice with *Kirchhoff coupling*.

6. The case of $m = 2$

The reader has noted already that the boundary conditions in the ST -form are not invariant with respect to the edge renumbering. Neglecting trivial lattice replacement corresponding to rotations and mirror images, we must distinguish two situations here:

- (i) Linearly independent columns of B are associated with parallel edges; without loss of generality we may suppose they are the “horizontal” ones. Then we apply the conditions in ST -form directly,

$$B = \begin{pmatrix} 1 & 0 & t_{11} & t_{12} \\ 0 & 1 & t_{21} & t_{22} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A = - \begin{pmatrix} s_{11} & s_{12} & 0 & 0 \\ \overline{s_{12}} & s_{22} & 0 & 0 \\ -\overline{t_{11}} & -\overline{t_{21}} & 1 & 0 \\ -\overline{t_{12}} & -\overline{t_{22}} & 0 & 1 \end{pmatrix},$$

where s_{11}, s_{22} are real and the other matrix entries are complex.

- (ii) Linearly independent columns of B can correspond also to mutually orthogonal edges, say, the left “horizontal” and the lower “vertical”. Then we use the conditions in a permuted form, with second and third row of $\Psi(0)$ and $\Psi'(0)$ interchanged. Since it is convenient to keep the entries order in these vectors, we interchange instead the second and the third column of the matrices A, B ,

$$B = \begin{pmatrix} 1 & t_{11} & 0 & t_{12} \\ 0 & t_{21} & 1 & t_{22} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A = - \begin{pmatrix} s_{11} & 0 & s_{12} & 0 \\ \overline{s_{12}} & 0 & s_{22} & 0 \\ -\overline{t_{11}} & 1 & -\overline{t_{21}} & 0 \\ -\overline{t_{12}} & 0 & -\overline{t_{22}} & 1 \end{pmatrix}.$$

However, since the spectral analysis of situations (i) and (ii) can be done in a very similar way, and moreover, also the structure of the spectral bands is essentially the same, we perform the analysis of the case (i) only.

The determinant in (10) leads to the spectral condition which can be written as

$$V_2 \cdot k^2 + V_1 \cdot k + V_0 = 0,$$

where V_2 , V_1 and V_0 are expressions depending on ak , on the entries of S , T , and on the quasimomentum components θ_1, θ_2 . By a direct computation we get

$$\begin{aligned} V_2 &= -4 \cos^2 ak \left[|t_{11}|^2 + |t_{22}|^2 + |t_{12}|^2 + |t_{21}|^2 \right] + 4 \sin^2 ak \left[1 + |t_{11}t_{22} - t_{12}t_{21}|^2 \right] \\ &\quad + 8 \cos ak \left[-\Re \left((t_{11}\overline{t_{21}} + t_{12}\overline{t_{22}})e^{i\theta_1} \right) + \Re \left((t_{22}\overline{t_{21}} + \overline{t_{11}}t_{12})e^{i\theta_2} \right) \right] \\ &\quad + 8\Re \left[t_{11}\overline{t_{22}}e^{i(\theta_1-\theta_2)} \right] + 8\Re \left[t_{12}\overline{t_{21}}e^{i(\theta_1+\theta_2)} \right] , \\ V_1 &= 4 \sin ak \left[-\cos ak \left(s_{11}(1 + |t_{22}|^2 + |t_{21}|^2) + s_{22}(1 + |t_{11}|^2 + |t_{12}|^2) \right. \right. \\ &\quad \left. \left. - 2\Re \left(s_{12}(\overline{t_{11}}t_{21} + \overline{t_{12}}t_{22}) \right) \right) \right. \\ &\quad \left. - 2\Re \left(s_{12}e^{i\theta_1} \right) + 2\Re \left((s_{11}\overline{t_{21}}t_{22} + s_{22}\overline{t_{11}}t_{12} - s_{12}\overline{t_{11}}t_{22} - s_{12}\overline{t_{12}}t_{21})e^{i\theta_2} \right) \right] , \\ V_0 &= -4 \sin^2 ak \cdot \det S . \end{aligned}$$

6.1. Linearly growing bands and gaps, or absence of gaps

If we divide the above spectral condition by k^2 , we can write it in the asymptotic form $V_2(ak) = \mathcal{O}(k^{-1})$, explicitly

$$\begin{aligned} &-4 \cos^2 ak \left[|t_{11}|^2 + |t_{22}|^2 + |t_{12}|^2 + |t_{21}|^2 \right] + 4 \sin^2 ak \left[1 + |t_{11}t_{22} - t_{12}t_{21}|^2 \right] \\ &\quad + 8 \cos ak \left[-\Re \left((t_{11}\overline{t_{21}} + t_{12}\overline{t_{22}})e^{i\theta_1} \right) + \Re \left((t_{22}\overline{t_{21}} + \overline{t_{11}}t_{12})e^{i\theta_2} \right) \right] \\ &\quad + 8\Re \left[t_{11}\overline{t_{22}}e^{i(\theta_1-\theta_2)} \right] + 8\Re \left[t_{12}\overline{t_{21}}e^{i(\theta_1+\theta_2)} \right] = \mathcal{O}(k^{-1}) , \end{aligned}$$

from which it is possible to obtain the “generic” spectral behaviour. Let us examine the *lhs* of the last relation. To this aim, we denote

$$\begin{aligned} K_c &:= 4 \left(|t_{11}|^2 + |t_{22}|^2 + |t_{12}|^2 + |t_{21}|^2 \right) \\ K_s &:= 4 \left(1 + |t_{11}t_{22} - t_{12}t_{21}|^2 \right) \\ L_c(\theta_1, \theta_2) &:= 8 \left[-\Re \left((t_{11}\overline{t_{21}} + t_{12}\overline{t_{22}})e^{i\theta_1} \right) + \Re \left((t_{22}\overline{t_{21}} + \overline{t_{11}}t_{12})e^{i\theta_2} \right) \right] \\ L(\theta_1, \theta_2) &:= 8\Re \left(t_{11}\overline{t_{22}}e^{i(\theta_1-\theta_2)} \right) + 8\Re \left(t_{12}\overline{t_{21}}e^{i(\theta_1+\theta_2)} \right) \end{aligned}$$

which allows us to write the coefficient $V_2 \equiv V_2(ak, \theta_1, \theta_2)$ as follows

$$V_2(x, \theta_1, \theta_2) = -K_c \cos^2 x + K_s \sin^2 x + \cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) .$$

To examine the spectral asymptotics, the following functions,

$$\begin{aligned} V_2^+(x) &:= \max \{ V_2(x, \theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} , \\ V_2^-(x) &:= \min \{ V_2(x, \theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} , \end{aligned}$$

will be essential, since the spectral condition can be expressed, up to an error of order of $\mathcal{O}(k^{-1})$, by the inequalities,

$$V_2^+(ak) > 0 \quad \wedge \quad V_2^-(ak) < 0 . \quad (16)$$

As we will see below, the following two constants will play an important role:

$$\begin{aligned} L_0^+ &:= 8 \max \left\{ \Re \left((t_{11}\overline{t_{21}} + t_{12}\overline{t_{22}})e^{i\theta_1} \right) + \Re \left((t_{22}\overline{t_{21}} + \overline{t_{11}}t_{12})e^{i\theta_2} \right) + \right. \\ &\quad \left. + \Re \left(t_{11}\overline{t_{22}}e^{i(\theta_1-\theta_2)} \right) + \Re \left(t_{12}\overline{t_{21}}e^{i(\theta_1+\theta_2)} \right) \mid \theta_1, \theta_2 \in (-\pi, \pi] \right\}, \\ L_{\frac{\pi}{2}}^- &:= 8 \min \left\{ \Re \left(t_{11}\overline{t_{22}}e^{i(\theta_1-\theta_2)} \right) + \Re \left(t_{12}\overline{t_{21}}e^{i(\theta_1+\theta_2)} \right) \mid \theta_1, \theta_2 \in (-\pi, \pi] \right\}; \end{aligned}$$

it is easy to see that $L_{\frac{\pi}{2}}^- = -8|t_{11}t_{22}| - 8|t_{12}t_{21}|$.

With this preliminary we are going to formulate and prove a claim which will be useful not only here, but also at other places further on.

Proposition 6.1. *Let*

$$F(\theta_1, \theta_2) = \Re(A_1 e^{i\theta_1}) + \Re(A_2 e^{i\theta_2}) + \Re(A_3 e^{i(\theta_1-\theta_2)}) + \Re(A_4 e^{i(\theta_1+\theta_2)}),$$

where the coefficients A_j , $j = 1, 2, 3, 4$, are independent of θ_1, θ_2 . Then the range of this expression, $\mathcal{F} := \{F(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi]\}$, is an interval which is non-degenerate if and only if there is an index $j \in \{1, 2, 3, 4\}$ such that $A_j \neq 0$.

Proof. Since F is continuous and $(-\pi, \pi]^2$ is connected, \mathcal{F} is an interval. To finish the proof it remains to check that a constant $C \in \mathbb{R}$ such that

$$F(\theta_1, \theta_2) = C \quad \text{for all } (\theta_1, \theta_2) \in (-\pi, \pi]^2 \quad (17)$$

exists if and only if $A_j = 0$ for all $j = 1, 2, 3, 4$.

Consider a fixed $\theta \in \mathbb{R}$ and a number $A \in \mathbb{C}$ such that $\arg A = \alpha$, then $\Re(Ae^{i\theta}) = \Re(|A|e^{i\alpha}e^{i\theta}) = |A|\cos(\alpha + \theta)$. We apply this idea to rewrite (17) as

$$|A_1|\cos(\alpha_1 + \theta_1) + |A_2|\cos(\alpha_2 + \theta_2) + |A_3|\cos(\alpha_3 + \theta_1 + \theta_2) + |A_4|\cos(\alpha_4 + \theta_1 - \theta_2) - C = 0$$

for all $(\theta_1, \theta_2) \in (-\pi, \pi]^2$. It is easy to see that the 5-tuple

$$1, \cos(\alpha_1 + \theta_1), \cos(\alpha_2 + \theta_2), \cos(\alpha_3 + \theta_1 + \theta_2), \cos(\alpha_4 + \theta_1 - \theta_2)$$

is a linearly independent set of functions on $[0, 2\pi)^2$, therefore (17) is satisfied if and only if $A_1 = A_2 = A_3 = A_4 = C = 0$. \square

To solve the spectral conditions (16), we need to know basic characteristics of the functions $V_2^+(x)$ and $V_2^-(x)$ involved in it.

Proposition 6.2. *The functions $V_2^+(x)$ and $V_2^-(x)$ have the following properties:*

(i) *Both $V_2^+(x)$, $V_2^-(x)$ are π -periodic and satisfy*

$$V_2^+\left(\frac{\pi}{2} - x\right) = V_2^+(x), \quad V_2^-\left(\frac{\pi}{2} - x\right) = V_2^-(x).$$

(ii) *Function $V_2^-(x)$ is increasing in $[0, \frac{\pi}{2}]$ and*

$$V_2^-(0) < 0, \quad V_2^-\left(\frac{\pi}{2}\right) = K_s + L_{\frac{\pi}{2}}^-.$$

(iii) It holds $V_2^+(0) = -K_c + L_0^+$, and there is a number $x_0 \in [0, \frac{\pi}{2}]$ such that

- V_2^+ is increasing in $[0, x_0]$,
- $V_2^+(x) > 0$ for all $x \in [x_0, \frac{\pi}{2}]$.

(iv) If at least two entries of T are nonzero, then $V_2^+(x) > V_2^-(x)$ for all $x \in (0, \frac{\pi}{2})$.

Proof of this proposition is technical and slightly long, and can be found in the appendix.

Using the above result we can characterize the spectrum.

Proposition 6.3. *If at least two entries of T are nonzero, then the following holds true:*

- If $L_0^+ > K_c$ and $L_{\frac{\pi}{2}}^- < -K_s$, there is a $k_0 > 0$ such that the interval $[k_0^2, +\infty)$ is in the spectrum.
- If $L_0^+ < K_c$, the spectrum has asymptotically gaps of the form

$$\left(\frac{n^2\pi^2}{a^2} - \frac{2bn\pi}{a^2} + \mathcal{O}(1), \frac{n^2\pi^2}{a^2} + \frac{2bn\pi}{a^2} + \mathcal{O}(1) \right),$$

where $b \in (0, \frac{\pi}{2})$ is the number uniquely determined by the condition $V_2^+(b) = 0$.

- If $L_{\frac{\pi}{2}}^- > -K_s$, the spectrum has asymptotically gaps of the form

$$\left(\left(n + \frac{1}{2} \right)^2 \frac{\pi^2}{a^2} - \frac{2cn\pi}{a^2} + \mathcal{O}(1), \left(n + \frac{1}{2} \right)^2 \frac{\pi^2}{a^2} + \frac{2cn\pi}{a^2} + \mathcal{O}(1) \right),$$

where $c \in (0, \frac{\pi}{2})$ is uniquely determined by the condition $V_2^-(\frac{\pi}{2} - c) = 0$.

Proof. The argument is based on Proposition 6.2 (i)-(iv). First we notice that if $L_0^+ > K_c$, then $V_2^+(x) > 0$ for all $x \in [0, \frac{\pi}{2}]$ according to (ii), and thus for all $x \in [0, +\infty)$ due to (i). Similarly, if $L_{\frac{\pi}{2}}^- < -K_s$, then $V_2^-(x) < 0$ for all $x \in [0, \frac{\pi}{2}]$ according to (iii), and thus for all $x \in [0, +\infty)$ due to (i). Consequently, for both $L_0^+ > K_c$ and $L_{\frac{\pi}{2}}^- < -K_s$, the asymptotic spectral condition (16) is satisfied for all k .

If $L_0^+ < K_c$, then by virtue of (ii) there is a $b \in (0, \frac{\pi}{2})$ such that $V_2^+(x) < 0$ on $[0, b]$ and $V_2^+(x) > 0$ on $(b, \frac{\pi}{2})$. Then the first inequality of (16) is not satisfied on $(0, \frac{b}{a})$, and we infer from (i) that it is not satisfied on each interval $(\frac{n\pi}{a} - \frac{b}{a}, \frac{n\pi}{a} + \frac{b}{a})$.

In the same vein, the inequality $L_{\frac{\pi}{2}}^- > -K_s$ in combination with (iii) implies existence of a $c \in (0, \frac{\pi}{2})$ such that $V_2^-(x) < 0$ on $[0, \frac{\pi}{2} - c)$ and $V_2^-(x) > 0$ on $(\frac{\pi}{2} - c, \frac{\pi}{2})$. The second inequality of (16) is then not satisfied on $(\frac{\pi}{2a} - \frac{c}{a}, \frac{\pi}{2a} + \frac{c}{a})$, and by (i) it is not satisfied on each interval $((n + \frac{1}{2}) \frac{\pi}{a} - \frac{c}{a}, (n + \frac{1}{2}) \frac{\pi}{a} + \frac{c}{a})$.

Finally, it follows from (iv) that if the matrix T has at least two non-vanishing entries, we have $b < \frac{\pi}{2} - c$ and the gaps cannot overlap asymptotically. \square

6.2. Further particular cases

Proposition 6.3 applies if at least two entries of T are nonzero. If this is not the case, the spectral condition simplifies significantly and one of the following situations occurs:

- $s_{12} = 0$. With such boundary conditions, the lattice is decomposed into separated edges or pairs of edges, and consequently the spectrum is pure point. As above in similar cases it is infinitely degenerate, of course, but the contribution from each edge pair has the usual semiclassical behaviour: the number of eigenvalues not exceeding k^2 has Weyl asymptotics with the leading term $\frac{a}{\pi}$.
- $s_{12} \neq 0$ and $T = 0$. The spectrum contains points $\frac{n^2\pi^2}{a^2}$ and bands of asymptotically constant width in the vicinity of $\frac{n^2\pi^2}{a^2}$; the points $\frac{n^2\pi^2}{a^2}$ may or may not lie in the bands. The gaps grows linearly as $n \rightarrow \infty$.
- $s_{12} \neq 0$ and $T \neq 0$. The spectrum asymptotically consists of bands located in the vicinity of the points $\left(\frac{n\pi}{a} + \frac{1}{2} \arccos \frac{1-|t|^2}{1+|t|^2}\right)^2$, where t is the nonzero entry of T . They are of asymptotically constant width while the gaps are linearly growing as the band index $n \rightarrow \infty$.

It remains to deal with the special cases $L_0^+ = K_c$, $L_{\frac{\pi}{2}}^- = -K_s$ left out in Proposition 6.3. We will not go into much detail here, but it is worth to solve this situation in the particular case of *scale-invariant coupling*, i.e. for $S = 0$. It turns out that:

- If $S = 0$ and $L_0^+ = K_c$, then there are no gaps around $\frac{n^2\pi^2}{a^2}$.
- If $S = 0$ and $L_{\frac{\pi}{2}}^- = -K_s$, then there are no gaps around $\left(n + \frac{1}{2}\right)^2 \frac{\pi^2}{a^2}$.

7. The case of $m = 3$

In this case we have a Hermitean S and complex numbers t_j determining

$$B = \begin{pmatrix} 1 & 0 & 0 & t_1 \\ 0 & 1 & 0 & t_2 \\ 0 & 0 & 1 & t_3 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A = - \begin{pmatrix} s_{11} & s_{12} & s_{13} & 0 \\ \overline{s_{12}} & s_{22} & s_{23} & 0 \\ \overline{s_{13}} & \overline{s_{23}} & s_{33} & 0 \\ -\overline{t_1} & -\overline{t_2} & -\overline{t_3} & 1 \end{pmatrix}.$$

In contrast to the previous case, there is no problem with the renumbering invariance, because the edge numbering can be changed if necessary by a trivial rotation of the lattice. A direct calculation of the determinant in (10) yields the spectral condition,

$$V_3 \cdot k^3 + V_2 \cdot k^2 + V_1 \cdot k + V_0 = 0,$$

where V_j , $j = 0, 1, 2, 3$, are expressions depending on ak , on the entries of the matrices S , T , and on the quasimomentum components θ_1, θ_2 , given explicitly by

$$\begin{aligned}
V_3 &= 4 \sin ak \left[(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak + 2\Re(t_1 \bar{t}_2 e^{i\theta_1}) - 2\Re(t_3 e^{i\theta_2}) \right], \\
V_2 &= 4 \cos^2 ak \left[-(s_{11} + s_{22}) (1 + |t_3|^2) - s_{33}(|t_1|^2 + |t_2|^2) + 2\Re((s_{13} \bar{t}_1 + s_{23} \bar{t}_2) t_3) \right] \\
&\quad + 4 \sin^2 ak \left[s_{11}|t_2|^2 + s_{22}|t_1|^2 + s_{33} - 2\Re(s_{12} \bar{t}_1 t_2) \right] \\
&\quad + 8 \cos ak \left[\Re((-s_{12} + \bar{s}_{23} t_1 \bar{t}_3 + s_{13} \bar{t}_2 t_3 - s_{12}|t_3|^2 - s_{33} t_1 \bar{t}_2) e^{i\theta_1}) \right. \\
&\quad \left. + \Re(((s_{11} + s_{22}) t_3 - \bar{s}_{13} t_1 - \bar{s}_{23} t_2) e^{i\theta_2}) \right] \\
&\quad + 8\Re((s_{12} t_3 - \bar{s}_{23} t_1) e^{i(\theta_1 + \theta_2)}) + 8\Re((s_{12} \bar{t}_3 - s_{13} \bar{t}_2) e^{i(\theta_1 - \theta_2)}) , \\
V_1 &= 4 \sin ak \cos ak \left[(|s_{12}|^2 - s_{11} s_{22})(1 + |t_3|^2) + (|s_{13}|^2 - s_{11} s_{33})(1 + |t_2|^2) \right. \\
&\quad \left. + (|s_{23}|^2 - s_{22} s_{33})(1 + |t_1|^2) + \right. \\
&\quad \left. + 2\Re((s_{12} s_{33} - s_{13} \bar{s}_{23}) \bar{t}_1 t_2) + 2\Re((s_{23} s_{11} - s_{13} \bar{s}_{12}) \bar{t}_2 t_3) + 2\Re((s_{13} s_{22} - s_{12} s_{23}) \bar{t}_1 t_3) \right] \\
&\quad + 8 \sin ak \cdot \Re((s_{13} \bar{s}_{23} - s_{33} s_{12}) e^{i\theta_1}) \\
&\quad + 8 \sin ak \cdot \Re\left[\left((\bar{s}_{12} \bar{s}_{23} - s_{22} \bar{s}_{13}) t_1 + (s_{12} \bar{s}_{13} - s_{11} \bar{s}_{23}) t_2 + (s_{11} s_{22} - |s_{12}|^2) t_3\right) e^{i\theta_2}\right], \\
V_0 &= -4 \sin^2 ak \cdot \det S.
\end{aligned}$$

The case $m = 3$ is probably the most interesting one. While in the one-dimensional case we have bands and gaps which are asymptotically either of constant width or linearly growing with the band index, a square lattice with $m = 3$ exhibits a considerably richer spectral behaviour. The bands are here of two types, mutually interlaced:

- “even” bands in the vicinity of $\frac{n^2 \pi^2}{a^2}$ with $n \in \mathbb{N}$,
- “odd” bands in the vicinity of $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$ with $n \in \mathbb{N}$,

In this section we focus on the generic situation, $|t_1| \neq |t_2|$ or $|t_3| \neq 1$, when we will be able to describe several interesting asymptotic types. The other possibility, $|t_1| = |t_2| \wedge |t_3| = 1$, will be briefly commented at the end.

Let us start with the spectral condition in the form $V_3 = \mathcal{O}(k^{-1})$, i.e.

$$4 \sin ak \left[(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak + 2\Re(t_1 \bar{t}_2 e^{i\theta_1}) - 2\Re(t_3 e^{i\theta_2}) \right] = \mathcal{O}(k^{-1}). \quad (18)$$

The *lhs* of the last equation should be close to zero for large k , which can be achieved either for small absolute value of $\sin ak$ or for small absolute value of the expression in the brackets. These possibilities refer to the “even” and “odd” bands mentioned above, respectively; they will be described in detail below. Unless stated otherwise, we suppose that $|t_1| \neq |t_2| \vee |t_3| \neq 1$.

7.1. Generic case: asymptotically constant spectral bands around $\frac{n^2\pi^2}{a^2}$

We start with the bands corresponding to small values of $|\sin ak|$. Let us consider the spectral condition in the form $V_3 + \frac{V_2}{k} = \mathcal{O}(k^{-2})$, divide it by four and rewrite it as

$$\begin{aligned} & \sin ak \left[(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak + 2\Re(t_1 \bar{t}_2 e^{i\theta_1}) - 2\Re(t_3 e^{i\theta_2}) \right. \\ & \quad \left. - \frac{\sin ak}{k} (s_{11}|t_2|^2 + s_{22}|t_1|^2 + s_{33} - 2\Re(s_{12} \bar{t}_1 t_2)) \right] \\ &= -\frac{\cos^2 ak}{k} \left[-(s_{11} + s_{22})(1 + |t_3|^2) - s_{33}(|t_1|^2 + |t_2|^2) + 2\Re((s_{13} \bar{t}_1 + s_{23} \bar{t}_2)t_3) \right] \\ & \quad - 2\frac{\cos ak}{k} \left[\Re((-s_{12} + \overline{s_{23}}t_1 \bar{t}_3 + s_{13} \bar{t}_2 t_3 - s_{12}|t_3|^2 - s_{23}t_1 \bar{t}_2)e^{i\theta_1}) \right. \\ & \quad \left. + \Re(((s_{11} + s_{22})t_3 - \overline{s_{13}}t_1 - \overline{s_{23}}t_2)e^{i\theta_2}) \right] \\ & \quad - \frac{2}{k} \Re((s_{12}t_3 - \overline{s_{23}}t_1)e^{i(\theta_1+\theta_2)}) - \frac{2}{k} \Re((s_{12} \bar{t}_3 - s_{13} \bar{t}_2)e^{i(\theta_1-\theta_2)}) + \mathcal{O}(k^{-2}). \quad (19) \end{aligned}$$

We restrict our considerations to the values of k such that $|\cos ak| > c$ where c is a constant satisfying $\frac{2(|t_1 t_2| + |t_3|)}{1 + |t_1|^2 + |t_2|^2 + |t_3|^2} < c < 1$; recall that such c exists in view of the initial assumption $|t_1| \neq |t_2| \vee |t_3| \neq 1$. Due to this restriction, the absolute value of the term in the brackets at the lhs of (19) can be asymptotically estimated from below by a positive constant, whence it is easy to see that high in the spectrum we have $\sin ak = \mathcal{O}(k^{-1})$. We set

$$k = \frac{n\pi}{a} + \frac{d}{n},$$

then $\sin ak = (-1)^n \cdot \frac{ad}{n} + \mathcal{O}(n^{-3})$, $\cos ak = (-1)^n + \mathcal{O}(n^{-2})$ and $\frac{1}{k} = \frac{a}{n\pi} + \mathcal{O}(n^{-2})$. We substitute from these relations into (19), divide both sides by the expression in the brackets at the lhs and after elementary manipulations we arrive at

$$\begin{aligned} & \frac{ad}{n} \cdot \left[(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) + 2(-1)^n \Re(t_1 \bar{t}_2 e^{i\theta_1}) - 2(-1)^n \Re(t_3 e^{i\theta_2}) \right] = \\ &= -\frac{a}{n\pi} \left[-(s_{11} + s_{22})(1 + |t_3|^2) - s_{33}(|t_1|^2 + |t_2|^2) + 2\Re((s_{13} \bar{t}_1 + s_{23} \bar{t}_2)t_3) \right] \\ & \quad - 2\frac{(-1)^n a}{n\pi} \left[\Re((-s_{12} + \overline{s_{23}}t_1 \bar{t}_3 + s_{13} \bar{t}_2 t_3 - s_{12}|t_3|^2 - s_{23}t_1 \bar{t}_2)e^{i\theta_1}) \right. \\ & \quad \left. + \Re(((s_{11} + s_{22})t_3 - \overline{s_{13}}t_1 - \overline{s_{23}}t_2)e^{i\theta_2}) \right] \\ & \quad - \frac{2a}{n\pi} \Re((s_{12}t_3 - \overline{s_{23}}t_1)e^{i(\theta_1+\theta_2)}) - \frac{2a}{n\pi} \Re((s_{12} \bar{t}_3 - s_{13} \bar{t}_2)e^{i(\theta_1-\theta_2)}) + \mathcal{O}(n^{-2}). \end{aligned}$$

We observe that all the terms $(-1)^n$ can be “absorbed” into θ_1 and θ_2 by the shift $(\theta_1, \theta_2) \mapsto (\theta_1 + n\pi, \theta_2 + n\pi)$, and thus neglected. Therefore the asymptotic condition can be written in the form

$$d = \frac{1}{\pi} \cdot \frac{-W_2(S, T, \theta_1, \theta_2)}{W_3(T, \theta_1, \theta_2)} + \mathcal{O}(n^{-1})$$

for

$$W_3(T, \theta_1, \theta_2) := (1 + |t_1|^2 + |t_2|^2 + |t_3|^2) + 2(-1)^n \Re(t_1 \bar{t}_2 e^{i\theta_1}) - 2(-1)^n \Re(t_3 e^{i\theta_2}),$$

$$\begin{aligned}
W_2(S, T, \theta_1, \theta_2) := & -(s_{11} + s_{22}) (1 + |t_3|^2) - s_{33}(|t_1|^2 + |t_2|^2) + 2\Re((s_{13}\bar{t}_1 + s_{23}\bar{t}_2)t_3) \\
& + 2\Re((-s_{12} + \overline{s_{23}}t_1\bar{t}_3 + s_{13}\bar{t}_2t_3 - s_{12}|t_3|^2 - s_{33}t_1\bar{t}_2)e^{i\theta_1}) \\
& + 2\Re(((s_{11} + s_{22})t_3 - \overline{s_{13}}t_1 - \overline{s_{23}}t_2)e^{i\theta_2}) \\
& + 2\Re((s_{12}t_3 - \overline{s_{23}}t_1)e^{i(\theta_1+\theta_2)}) + 2\Re((s_{12}\bar{t}_3 - s_{13}\bar{t}_2)e^{i(\theta_1-\theta_2)}) .
\end{aligned}$$

Now we denote

$$\mathcal{D} := \left\{ \frac{-W_2(S, T, \theta_1, \theta_2)}{W_3(T, \theta_1, \theta_2)} \mid \theta_1, \theta_2 \in (-\pi, \pi] \right\} ;$$

note that \mathcal{D} is an interval which is bounded due to the condition $|t_1| \neq |t_2| \vee |t_3| \neq 1$. The spectral bands are then described in terms of \mathcal{D} as follows,

$$k = \frac{n\pi}{a} + \frac{d}{n\pi} + \mathcal{O}(n^{-2}), \quad d \in \mathcal{D}, \quad (20)$$

which yields the allowed energy values

$$k^2 = \frac{n^2\pi^2}{a^2} + 2\frac{d}{a} + \mathcal{O}(n^{-1}), \quad d \in \mathcal{D}.$$

Consequently, these bands are of asymptotically constant width as $n \rightarrow \infty$.

Furthermore, it is easy to show that if

- (a) $T = 0$ and $s_{12} = 0$, or
- (b) $t_1t_2 = 0$, $t_3 = 0$ and S is diagonal,

then the fraction $\frac{-W_2(S, T, \theta_1, \theta_2)}{W_3(T, \theta_1, \theta_2)}$ is independent of (θ_1, θ_2) , and thus the interval \mathcal{D} shrinks to a point. These cases need a special approach.

One can check that (b) refers to the situation when the lattice is decomposed either to individual edges (if $T = 0$) or to pairs of edges (if $T \neq 0$), with infinitely degenerate eigenvalues in the vicinity of $(\frac{n\pi}{a})^2$. The case (a) is much more interesting and we will analyze it below.

7.2. Spectral bands around $\frac{n^2\pi^2}{a^2}$ shrinking as n^{-2}

Under the assumptions of the case (a) above the spectral condition simplifies to

$$\begin{aligned}
& 4k^3 \sin ak \cos ak + 4k^2 [-(s_{11} + s_{22}) \cos^2 ak + s_{33} \sin^2 ak] \\
& + 4k \sin ak [(|s_{13}|^2 + |s_{23}|^2 - s_{11}s_{22} - (s_{11} + s_{22})s_{33}) \cos ak + 2\Re(s_{13}\overline{s_{23}}e^{i\theta_1})] \\
& - 4 \sin^2 ak \cdot \det S = 0.
\end{aligned}$$

The spectrum is given by (20) with $\mathcal{D} = \{\frac{a}{\pi}(s_{11} + s_{22})\}$. Since the latter is a one-point set, the spectral band is determined by the next term in the expansion. We set

$$k = \frac{n\pi}{a} + \frac{a}{n\pi}(s_{11} + s_{22}) + \frac{d'}{n^2},$$

and performing a calculation similar to that of Sec. 7.1, we arrive at the expression for d' . Surprisingly, d' itself behaves like n^{-1} , i.e. the last term above is of order of $\mathcal{O}(n^{-3})$,

$$\frac{d'}{n^2} = \frac{a(s_{11} + s_{22})}{n^3\pi^3} \left[-(s_{11} + s_{22}) + a \left(\frac{s_{11}^2 + s_{22}^2}{2} + 2s_{11}s_{22} + |s_{13}|^2 + |s_{23}|^2 \right) - 2a\Re(s_{13}\overline{s_{23}}e^{i\theta_1}) \right].$$

Thus k^2 belongs asymptotically to the spectrum if

$$k = \frac{n\pi}{a} + \frac{s_{11} + s_{22}}{n\pi} + \frac{a(s_{11} + s_{22})}{n^3\pi^3} \left[-(s_{11} + s_{22}) + a \left(\frac{s_{11}^2 + s_{22}^2}{2} + 2s_{11}s_{22} + |s_{13}|^2 + |s_{23}|^2 \right) \right] \\ + \frac{2a^2}{n^3\pi^3} |s_{11} + s_{22}| \cdot |s_{13}s_{23}| \cos \vartheta + \mathcal{O}(n^{-4}) \quad \text{for } \vartheta \in [0, 2\pi).$$

The left and right endpoint of the spectral band are then given as k_L^2 and k_R^2 with $\vartheta_L = \pi$ and $\vartheta_R = 0$, respectively, hence the band width behaves like

$$k_R^2 - k_L^2 = (k_R - k_L)(k_R + k_L) = 8 \frac{a}{n^2\pi^2} |s_{11} + s_{22}| \cdot |s_{13}s_{23}| + \mathcal{O}(n^{-3})$$

in the asymptotic regime, $n \rightarrow \infty$.

Note that there are two exceptional cases here, namely:

- $s_{13} = 0$ or $s_{23} = 0$. The spectral condition is independent of θ_1, θ_2 , thus it has only point solutions.
- $s_{11} + s_{22} = 0$. The spectral condition factorizes, $\sin ak [\cos ak + \mathcal{O}(\frac{1}{k})] = 0$, producing no (true) band in the vicinity of $\frac{n^2\pi^2}{a^2}$.

7.3. Generic case: linearly growing spectral bands around $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$

Now we proceed to the “odd” bands, i.e. those corresponding to asymptotically small values of the expression $|(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak + 2\Re(t_1\overline{t_2}e^{i\theta_1}) - 2\Re(t_3e^{i\theta_2})|$. Their structure can be derived directly from the spectral condition (18), we just replace for the sake of simplicity the term $2\Re(t_1\overline{t_2}e^{i\theta_1}) - 2\Re(t_3e^{i\theta_2})$ by $2(|t_1t_2| + |t_3|) \cos \vartheta$ in analogy with what we did in Section 5.2, cf. Observation 5.1:

$$4 \sin ak [(1 + |t_1|^2 + |t_2|^2 + |t_3|^2) \cos ak + 2(|t_1t_2| + |t_3|) \cos \vartheta] = \mathcal{O}(k^{-1})$$

Suppose that $|t_1t_2| + |t_3| \neq 0$ (the case $t_1t_2 = t_3 = 0$ is postponed to Sec. 7.4 below), then we may divide the equation by $8(|t_1\overline{t_2}| + |t_3|)$ obtaining

$$\sin ak \left[\frac{1 + |t_1|^2 + |t_2|^2 + |t_3|^2}{2(|t_1t_2| + |t_3|)} \cos ak + \cos \vartheta \right] = \mathcal{O}(k^{-1}). \quad (21)$$

Since the situation when $|\sin ak|$ is very small has been treated in the part devoted to “even” bands, here we adopt the premise that $|\sin ak|$ is large enough. More precisely, we restrict our considerations to such values k that $|\sin ak| > c$, where c is a constant satisfying $0 < c < 1$, the exact value plays no role. Then (21) can be rewritten as

$$\cos \vartheta = \frac{1 + |t_1|^2 + |t_2|^2 + |t_3|^2}{2(|t_1t_2| + |t_3|)} \cos ak + \mathcal{O}(k^{-1}).$$

Such a condition has a solution for some parameter ϑ if the modulus of the rhs rhs is smaller than one, i.e. for

$$|\cos ak| < \frac{2(|t_1 t_2| + |t_3|)}{1 + |t_1|^2 + |t_2|^2 + |t_3|^2} + \mathcal{O}(k^{-1}). \quad (22)$$

In analogy with Sec. 5.2, we infer that the spectral bands are neighbourhoods of the points $\left[(n + \frac{1}{2}) \frac{\pi}{a}\right]^2$. We set $k = (n + \frac{1}{2}) \frac{\pi}{a} + d$, thus $|\cos ak| = |\sin ad|$ and $\frac{1}{k}$ of the n -th band solution is $\mathcal{O}(n^{-1})$. Then (22) can be rewritten as

$$|\sin ad| < \frac{2(|t_1 t_2| + |t_3|)}{1 + |t_1|^2 + |t_2|^2 + |t_3|^2} + \mathcal{O}(n^{-1}).$$

Recall that it follows from the initial assumption $|t_1| \neq |t_2| \vee |t_3| \neq 1$ that the first term at the rhs is smaller than one, cf. Observation 5.1, hence it makes sense to set $\Delta := \arcsin \frac{2(|t_1 t_2| + |t_3|)}{1 + |t_1|^2 + |t_2|^2 + |t_3|^2} \in (0, \frac{\pi}{2})$. The spectral bands are then given by

$$\left(\left(n + \frac{1}{2}\right)^2 \frac{\pi^2}{a^2} - 2 \frac{n\pi}{a^2} \Delta + \mathcal{O}(1), \left(n + \frac{1}{2}\right)^2 \frac{\pi^2}{a^2} + 2 \frac{n\pi}{a^2} \Delta + \mathcal{O}(1) \right),$$

in the high-energy asymptotics, $n \rightarrow \infty$.

7.4. Asymptotically constant spectral bands at $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$

Let the matrix T satisfy $t_1 t_2 = t_3 = 0$. We may suppose without loss of generality that $t_2 = 0$. The substitution $t_3 = t_2 = 0$ into the spectral condition $V_3 + \frac{V_2}{k} = \mathcal{O}(k^{-2})$ gives

$$\begin{aligned} \sin ak \cos ak (1 + |t_1|^2) &= \frac{\cos^2 ak}{k} (s_{11} + s_{22} + s_{33}|t_1|^2) - \frac{\sin^2 ak}{k} (s_{22}|t_1|^2 + s_{33}) \\ &+ \frac{2 \cos ak}{k} [\Re(s_{12}e^{i\theta_1}) + \Re(\overline{s_{13}}t_1e^{i\theta_2})] + \frac{2}{k} \Re(t_1 \overline{s_{23}}e^{i(\theta_1+\theta_2)}) + \mathcal{O}(k^{-2}). \end{aligned} \quad (23)$$

We proceed in a way analogous to Sec. 7.1 setting $k = (n + \frac{1}{2}) \frac{\pi}{a} + \delta$ and substituting the expansions

$$\cos ak = -(-1)^n \cdot a\delta + \mathcal{O}(\delta^3), \quad \sin ak = (-1)^n + \mathcal{O}(\delta^2), \quad \frac{1}{k} = \frac{a}{n\pi} + \mathcal{O}(n^{-2})$$

into (23), which yields after a simple manipulation an expression for δ ,

$$\delta = \frac{1}{n\pi} \cdot \left[-\frac{s_{22}|t_1|^2 + s_{33}}{1 + |t_1|^2} + \frac{2}{1 + |t_1|^2} \Re(t_1 \overline{s_{23}}e^{i(\theta_1+\theta_2)}) \right] + \mathcal{O}(n^{-2}).$$

Hence the spectral bands are determined by the values of k satisfying

$$k = \left(n + \frac{1}{2}\right) \frac{\pi}{a} - \frac{1}{n\pi} \cdot \frac{s_{22}|t_1|^2 + s_{33}}{1 + |t_1|^2} + \frac{1}{n\pi} \cdot \frac{2|t_1 s_{23}|}{1 + |t_1|^2} \cos \vartheta + \mathcal{O}(n^{-2})$$

so that

$$k^2 = \left(n + \frac{1}{2}\right)^2 \frac{\pi^2}{a^2} + \frac{2}{a} \cdot \frac{s_{22}|t_1|^2 + s_{33}}{1 + |t_1|^2} + \frac{2}{a} \cdot \frac{2|t_1 s_{23}|}{1 + |t_1|^2} \cos \vartheta + \mathcal{O}(n^{-1}), \quad \vartheta \in [0, 2\pi).$$

giving rise to asymptotically constant-width bands.

Note that the leading “band-producing” term may collapse to a single point which happens if $t_1 = 0$ or $s_{23} = 0$. The first named situation will be discussed in detail in Sections 7.5–7.7, the second one will be omitted, since the analysis is in principle similar.

7.5. Spectral bands at $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$ shrinking as n^{-1}

The bands in the vicinity of $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$ may shrink as n^{-1} provided the matrices S and T satisfy certain conditions in addition to $t_2 = t_3 = 0$, namely $t_1 = 0$ and $s_{13}s_{23} \neq 0$. We will demonstrate this fact in the first case, $t_1 = 0$.

We proceed as in Sec. 7.4, but we take one more term in the expansion of k , i.e. we set

$$k = \left(n + \frac{1}{2}\right) \frac{\pi}{a} + \frac{s_{33}}{n\pi} + \delta,$$

and substitute into the spectral condition in the form $V_3 + \frac{V_2}{k} + \frac{V_1}{k^2} = \mathcal{O}(k^{-3})$. A calculation leads to the expression $\delta = \frac{1}{n^2} \left[-\frac{s_{33}}{2\pi} + \frac{2a}{\pi^2} \Re((s_{13}\bar{s}_{23})e^{i\theta_1}) \right]$ in the leading order, hence

$$k = \left(n + \frac{1}{2}\right) \frac{\pi}{a} + \frac{s_{33}}{n\pi} - \frac{s_{33}}{2n^2\pi} + \frac{2a}{n^2\pi^2} |s_{13}s_{23}| \cos \vartheta + \mathcal{O}(n^{-3}), \quad \vartheta \in [0, 2\pi).$$

The band edges correspond to $\vartheta_L = \pi, 0$, respectively, and the band width equals

$$\frac{8}{n\pi} |s_{13}s_{23}| + \mathcal{O}(n^{-2}),$$

i.e. the bands shrink asymptotically as n^{-1} unless $s_{13} = 0$ or $s_{23} = 0$ – these cases will be discussed in the following sections.

7.6. Spectral bands at $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$ shrinking as n^{-2}

If $T = 0$ and $s_{23} = 0$, the following spectral band asymptotics can be derived,

$$k = \left(n + \frac{1}{2}\right) \frac{\pi}{a} + \frac{s_{33}}{n\pi} - \frac{s_{33}}{2n^2\pi} + \frac{\mathcal{C}}{n^3} - \frac{a}{n^3} \cdot \frac{s_{33}}{\pi^2} |s_{12}| \cos \vartheta + \mathcal{O}(n^{-4}), \quad \vartheta \in [0, 2\pi),$$

where \mathcal{C} depends only on S and a . This determines bands of the widths

$$\frac{4}{n^2\pi} |s_{33}s_{12}| + \mathcal{O}(n^{-3}),$$

i.e. they shrink asymptotically as n^{-2} providing that $s_{33} \neq 0$ and $s_{12} \neq 0$.

Remark 7.1. If $T = 0$, $s_{23} = 0$ and $s_{12} = 0$, the spectral condition is independent of θ_1, θ_2 , thus the spectrum is pure point.

7.7. Spectral bands at $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$ shrinking as n^{-3}

Let $T = 0$ and $s_{23} = s_{33} = 0$. Then the spectral bands are characterized by the following asymptotical condition,

$$k = \left(n + \frac{1}{2}\right) \frac{\pi}{a} - \frac{a^2}{n^3} \cdot \frac{|s_{13}|^2 s_{22}}{\pi^3} + \frac{a^2}{n^4} \cdot \frac{3|s_{13}|^2 s_{22}}{2\pi^3} + \frac{a^3}{n^4} \cdot \frac{2|s_{13}|^2 s_{22}}{2\pi^4} |s_{12}| \cos \vartheta + \mathcal{O}(n^{-5})$$

with $\vartheta \in [0, 2\pi)$, thus the band widths are given by

$$8 \frac{a^2}{n^3} \cdot \frac{|s_{13}|^2 s_{22}}{2\pi^3} |s_{12}| \cos \vartheta + \mathcal{O}(n^{-4}),$$

i.e. they shrink asymptotically as n^{-3} providing $s_{12} \neq 0$, $s_{13} \neq 0$ and $s_{22} \neq 0$.

Remark 7.2. Let $T = 0$, $s_{23} = 0$ and $s_{33} = 0$. Then:

- If $s_{12} = 0$, the spectral condition is independent of the quasimomentum components θ_1, θ_2 so the spectrum is pure point.
- If $s_{13} = 0$ or $s_{22} = 0$, the spectral condition can be factorized in the form $\cos ak \cdot [\sin ak + \mathcal{O}(\frac{1}{n})]$, and consequently, the band in the vicinity of $(n + \frac{1}{2})^2 \frac{\pi^2}{a^2}$ collapses into a single point.

7.8. The particular case $|t_1| = |t_2| \wedge |t_3| = 1$

This situation will not be treated in detail, but we will comment on the prominent case $S = 0$ which corresponds to the *scale-invariant vertex coupling*. If S vanishes, the spectral condition simplifies to $V_3 = 0$ which can be rewritten as

$$4 \sin ak [(2 + 2|t_1|^2) \cos ak - 2|t_1|^2 \cos \vartheta_1 - 2 \cos \vartheta_2] = 0,$$

where ϑ_1 and ϑ_2 are properly shifted θ_1, θ_2 . The choice $\vartheta_1 = \vartheta_2 = ak$ sets the expression in the brackets to zero, therefore the spectrum contains the positive halfline.

8. The case of $m = 4$

Finally, we pass to the case which is generic from the viewpoint of the boundary condition (1) when the matrix B is regular. Following the discussion in the opening we set

$$B = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad A = - \begin{pmatrix} s_{11} & s_{12} & s_{13} & s_{14} \\ \overline{s_{12}} & s_{22} & s_{23} & s_{24} \\ \overline{s_{13}} & \overline{s_{23}} & s_{33} & s_{34} \\ \overline{s_{14}} & \overline{s_{24}} & \overline{s_{34}} & s_{44} \end{pmatrix}$$

There is obviously no problem with the renumbering the lattice edges. A direct calculation of the determinant in (10) leads to the spectral condition

$$V_4 \cdot k^4 + V_3 \cdot k^3 + V_2 \cdot k^2 + V_1 \cdot k + V_0 = 0,$$

where V_j , $j = 0, 1, 2, 3, 4$, are expressions depending on ak , on entries of the matrix S , and on the quasimomentum components θ_1, θ_2 , given by the formulæ

$$\begin{aligned}
V_4 &= -4 \sin^2 ak, \\
V_3 &= 4 \sin ak \left[(s_{11} + s_{22} + s_{33} + s_{44}) \cos ak + 2\Re(s_{12}e^{i\theta_1}) + 2\Re(s_{34}e^{i\theta_2}) \right], \\
V_2 &= 4 \cos^2 ak \left(|s_{13}|^2 - s_{11}s_{33} + |s_{14}|^2 - s_{11}s_{44} + |s_{23}|^2 - s_{22}s_{33} + |s_{24}|^2 - s_{22}s_{44} \right) + \\
&\quad + 4 \sin^2 ak \left(s_{11}s_{22} - |s_{12}|^2 + s_{33}s_{44} - |s_{34}|^2 \right) \\
&\quad + 8 \cos ak \left[-(s_{33} + s_{44}) \cdot \Re(s_{12}e^{i\theta_1}) + \Re((s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}})e^{i\theta_1}) \right. \\
&\quad \left. - (s_{11} + s_{22}) \cdot \Re(s_{34}e^{i\theta_2}) + \Re((\overline{s_{13}}s_{14} + \overline{s_{23}}s_{24})e^{i\theta_2}) \right] \\
&\quad + 8\Re[(s_{14}\overline{s_{23}} - s_{12}s_{34})e^{i(\theta_1+\theta_2)}] + 8\Re[(s_{13}\overline{s_{24}} - s_{12}\overline{s_{34}})e^{i(\theta_1-\theta_2)}], \\
V_0 &= -4 \sin^2 ak \cdot \det S.
\end{aligned}$$

The remaining term V_1 will not be needed – it is sufficient to know that it is bounded with respect to the parameters. The spectral condition can be written as

$$\begin{aligned}
\sin^2 ak &= \frac{\sin ak}{k} \cdot \left[(s_{11} + s_{22} + s_{33} + s_{44}) \cos ak + 2\Re(s_{12}e^{i\theta_1}) + 2\Re(s_{34}e^{i\theta_2}) \right] \\
&\quad + \frac{\cos^2 ak}{k^2} \left(|s_{13}|^2 - s_{11}s_{33} + |s_{14}|^2 - s_{11}s_{44} + |s_{23}|^2 - s_{22}s_{33} + |s_{24}|^2 - s_{22}s_{44} \right) \\
&\quad + \frac{2 \cos ak}{k^2} \left[-(s_{33} + s_{44}) \cdot \Re(s_{12}e^{i\theta_1}) + \Re((s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}})e^{i\theta_1}) \right. \\
&\quad \left. - (s_{11} + s_{22}) \cdot \Re(s_{34}e^{i\theta_2}) + \Re((\overline{s_{13}}s_{14} + \overline{s_{23}}s_{24})e^{i\theta_2}) \right] \\
&\quad + \frac{2}{k^2} \Re \left[((s_{14}\overline{s_{23}} - s_{12}s_{34})e^{i(\theta_1+\theta_2)}) + 8\Re((s_{13}\overline{s_{24}} - s_{12}\overline{s_{34}})e^{i(\theta_1-\theta_2)}) \right] \\
&\quad + \frac{\sin^2 ak}{k^2} \left(s_{11}s_{22} - |s_{12}|^2 + s_{33}s_{44} - |s_{34}|^2 \right) \\
&\quad + \mathcal{O}(k^{-3}).
\end{aligned} \tag{24}$$

Since the *rhs* is of the order of $\mathcal{O}(k^{-2})$, it follows that the values of k that solve the spectral condition are asymptotically close to the points $\frac{n\pi}{a}$, $n \in \mathbb{N}$. With this fact in mind it is convenient to express k introducing d such that

$$k = \frac{n\pi}{a} + \frac{d}{n\pi}. \tag{25}$$

Substituting this into (24), we get after a simple manipulation,

$$\begin{aligned}
d^2 - d \cdot &\left[s_{11} + s_{22} + s_{33} + s_{44} + 2 \cdot (-1)^n \cdot \Re(s_{12}e^{i\theta_1}) + 2 \cdot (-1)^n \cdot \Re(s_{34}e^{i\theta_2}) \right] \\
&- \left(|s_{13}|^2 - s_{11}s_{33} + |s_{14}|^2 - s_{11}s_{44} + |s_{23}|^2 - s_{22}s_{33} + |s_{24}|^2 - s_{22}s_{44} \right) \\
&- 2 \cdot (-1)^n \cdot \left[-(s_{33} + s_{44}) \cdot \Re(s_{12}e^{i\theta_1}) + \Re((s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}})e^{i\theta_1}) \right. \\
&\quad \left. - (s_{11} + s_{22}) \cdot \Re(s_{34}e^{i\theta_2}) + \Re((\overline{s_{13}}s_{14} + \overline{s_{23}}s_{24})e^{i\theta_2}) \right] \\
&- 2\Re[(s_{14}\overline{s_{23}} - s_{12}s_{34})e^{i(\theta_1+\theta_2)}] - 2\Re[(s_{13}\overline{s_{24}} - s_{12}\overline{s_{34}})e^{i(\theta_1-\theta_2)}] = \mathcal{O}(n^{-1}). \tag{26}
\end{aligned}$$

We observe that the last relation has the structure

$$d^2 + 2p \cdot d + q = \mathcal{O}(n^{-1}) \quad (27)$$

with the quantities p, q depending only on S, θ_1, θ_2 and the sign of n . A value $k^2 > 0$ with k of the form (25) belongs to the spectrum if there are θ_1, θ_2 such that the above condition is satisfied. The solutions of (27) are given by

$$d_{1,2} = -p \pm \sqrt{p^2 - q} + \mathcal{O}(n^{-1}). \quad (28)$$

Proposition 8.1. *It holds $\max\{p^2 - q \mid \theta_1, \theta_2 \in (-\pi, \pi]\} \geq 0$.*

Proof. Taking the value of q from (26) and p^2 arranged into the form

$$p^2 = \frac{1}{4}(s_{11} + s_{22} - s_{33} - s_{44})^2 + (s_{11}s_{33} + s_{11}s_{44} + s_{22}s_{33} + s_{22}s_{44}) + (-1)^n \cdot (s_{11} + s_{22} + s_{33} + s_{44}) [\Re(s_{12}e^{i\theta_1}) + \Re(s_{34}e^{i\theta_2})] + [\Re(s_{12}e^{i\theta_1}) + \Re(s_{34}e^{i\theta_2})]^2,$$

we find

$$\begin{aligned} p^2 - q &= \frac{1}{4}(s_{11} + s_{22} - s_{33} - s_{44})^2 + [\Re(s_{12}e^{i\theta_1}) - \Re(s_{34}e^{i\theta_2})]^2 \\ &\quad + (-1)^n \cdot \Re[(s_{11} + s_{22} - s_{33} - s_{44})s_{12} + 2(s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}})]e^{i\theta_1} \\ &\quad + (-1)^n \cdot \Re[(-s_{11} - s_{22} + s_{33} + s_{44})s_{34} + 2(\overline{s_{13}}s_{14} + \overline{s_{23}}s_{24})]e^{i\theta_2} \\ &\quad + |s_{14}|^2 + |s_{23}|^2 + 2\Re(s_{14}\overline{s_{23}}e^{i(\theta_1+\theta_2)}) + |s_{13}|^2 + |s_{24}|^2 + 2\Re(s_{13}\overline{s_{24}}e^{i(\theta_1-\theta_2)}). \end{aligned} \quad (29)$$

It obviously holds

$$\begin{aligned} |s_{14}|^2 + |s_{23}|^2 + 2\Re(s_{14}\overline{s_{23}}e^{i(\theta_1+\theta_2)}) &\geq (|s_{14}| - |s_{23}|)^2 \geq 0, \\ |s_{13}|^2 + |s_{24}|^2 + 2\Re(s_{13}\overline{s_{24}}e^{i(\theta_1-\theta_2)}) &\geq (|s_{13}| - |s_{24}|)^2 \geq 0, \end{aligned}$$

and θ_1, θ_2 can be chosen so that the terms on the second and third line of (29) are non-negative. Therefore

$$\begin{aligned} \max\{p^2 - q \mid \theta_1, \theta_2 \in (-\pi, \pi]\} \\ \geq \frac{1}{4}(s_{11} + s_{22} - s_{33} - s_{44})^2 + (|s_{14}| - |s_{23}|)^2 + (|s_{13}| - |s_{24}|)^2 \geq 0, \end{aligned}$$

which we have set up to prove. \square

Corollary 8.2. *If $\max\{p^2 - q \mid \theta_1, \theta_2 \in (-\pi, \pi]\} = 0$, then $S = \text{diag}(s_{11}, s_{22}, s_{33}, s_{44})$ and $s_{11} + s_{22} - s_{33} - s_{44} = 0$.*

Proof. It follows from the last part of the previous proof that the premise requires $s_{11} + s_{22} - s_{33} - s_{44} = 0$. If we substitute this into *rhs* of (29) and make the same estimate as in the proof, we infer $s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}} = 0$, $\overline{s_{13}}s_{14} + \overline{s_{23}}s_{24} = 0$. Then θ_1, θ_2 can be obviously chosen such that $p^2 - q = (|s_{14}| + |s_{23}|)^2 + (|s_{13}| + |s_{24}|)^2$, hence necessarily $s_{14} = s_{23} = s_{13} = s_{24} = 0$. Now (29) gives $p^2 - q = [\Re(s_{12}e^{i\theta_1}) - \Re(s_{34}e^{i\theta_2})]^2$ which does not exceed zero only if $s_{12} = s_{34} = 0$. \square

8.1. Point spectrum for a diagonal matrix S

If $m = 4$ and all the off-diagonal entries of S vanish, then the boundary conditions (4) describe the system of decoupled edges of the length a . Such system has a point spectrum which is not difficult to find. We have two edges types:

- “horizontal”, with the boundary conditions $\psi'(0) = s_{22}\psi(0)$, $\psi'(a) = -s_{11}\psi(a)$,
- “vertical”, with the boundary conditions $\psi'(0) = s_{44}\psi(0)$, $\psi'(a) = -s_{33}\psi(a)$.

The corresponding spectral conditions are

$$(s_{1+2j,1+2j} + ks_{2+2j,2+2j}) \cos ka = (k - s_{1+2j,1+2j}s_{2+2j,2+2j}) \sin ka, \quad j = 0, 1.$$

Their solutions are thus

$$k = \frac{n\pi}{a} + \frac{\arctg s_{2+2j,2+2j}}{a} + \frac{s_{1+2j,1+2j}}{n\pi} + \mathcal{O}(n^{-2}), \quad j = 0, 1,$$

giving rise the eigenvalues, or flat bands of the lattice Hamiltonian,

$$k^2 = \left(\frac{n\pi}{a}\right)^2 + 2 \frac{n\pi \arctg s_{2+2j,2+2j}}{a^2} + \left(\frac{\arctg s_{2+2j,2+2j}}{a}\right)^2 + 2 \frac{s_{1+2j,1+2j}}{a} + \mathcal{O}(n^{-2})$$

for $j = 0, 1$ corresponding the two edge orientations.

8.2. A general matrix S

Let us next consider the following sets related to solutions to condition (28),

$$\mathcal{D}_{1,2} = \{-p \pm \sqrt{p^2 - q} \mid \theta_1, \theta_2 \in (-\pi, \pi]\} \cap \mathbb{R},$$

It follows from Proposition 8.1 that $\mathcal{D}_1 \neq \emptyset \neq \mathcal{D}_2$. We will show now that if one of them contains more than one point, then both contain a non-degenerated interval.

Proposition 8.3. *Let one of the expressions $-p + \sqrt{p^2 - q}$, $-p - \sqrt{p^2 - q}$ be independent of (θ_1, θ_2) , then the same is true for the other one.*

Proof. Let us suppose that $-p + \sqrt{p^2 - q} = c$ with $c \in \mathbb{R}$ holds for (θ_1, θ_2) . In such a case $\sqrt{p^2 - q} = p + c$, hence $-q - 2pc = c^2$, in other words, the expression $-q - 2pc$ is independent of (θ_1, θ_2) . Since

$$\begin{aligned} -q - 2pc &= (|s_{13}|^2 - s_{11}s_{33} + |s_{14}|^2 - s_{11}s_{44} + |s_{23}|^2 - s_{22}s_{33} + |s_{24}|^2 - s_{22}s_{44}) \\ &\quad + 2 \cdot (-1)^n \cdot [-(s_{33} + s_{44}) \cdot \Re(s_{12}e^{i\theta_1}) + \Re((s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}})e^{i\theta_1}) \\ &\quad - (s_{11} + s_{22}) \cdot \Re(s_{34}e^{i\theta_2}) + \Re((\overline{s_{13}}s_{14} + \overline{s_{23}}s_{24})e^{i\theta_2})] \\ &\quad + 2\Re[(s_{14}\overline{s_{23}} - s_{12}s_{34})e^{i(\theta_1+\theta_2)}] + 2\Re[(s_{13}\overline{s_{24}} - s_{12}\overline{s_{34}})e^{i(\theta_1-\theta_2)}] \\ &\quad + c \cdot [s_{11} + s_{22} + s_{33} + s_{44} + 2 \cdot (-1)^n \cdot \Re(s_{12}e^{i\theta_1}) + 2 \cdot (-1)^n \cdot \Re(s_{34}e^{i\theta_2})], \end{aligned}$$

we easily find that also the expression

$$\begin{aligned} & (-1)^n \cdot \Re \left[((-(s_{33} + s_{44}) + c) \cdot s_{12} + s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}}) e^{i\theta_1} \right] \\ & (-1)^n \cdot \Re \left[((-(s_{11} + s_{22}) + c) \cdot s_{34} + \overline{s_{13}}s_{14} + \overline{s_{23}}s_{24}) e^{i\theta_2} \right] \\ & + \Re \left[(s_{14}\overline{s_{23}} - s_{12}s_{34}) e^{i(\theta_1+\theta_2)} \right] + \Re \left[(s_{13}\overline{s_{24}} - s_{12}\overline{s_{34}}) e^{i(\theta_1-\theta_2)} \right] \end{aligned}$$

should be independent of (θ_1, θ_2) . It follows from Proposition 6.1 that this is true if and only if the whole expression identically equals zero. This in turn means that the *lhs* of the condition (27) is independent of θ_1, θ_2 , and consequently, both roots of the equation $d^2 + 2pd + q = 0$ are independent of θ_1, θ_2 . \square

Proposition 8.3 in fact says that only two situations are possible, either both sets $\mathcal{D}_1, \mathcal{D}_2$ are non-degenerate intervals, or each of them contains a single element only.

Proposition 8.4. *The sets $\mathcal{D}_1, \mathcal{D}_2$ are single-element sets iff at most one pair of off-diagonal elements of S is nonzero, and moreover, $s_{12} = s_{34} = 0$.*

Proof. $\mathcal{D}_1, \mathcal{D}_2$ are one-element iff both $-p + \sqrt{p^2 - q}$, $-p - \sqrt{p^2 - q}$ are independent of θ_1, θ_2 , and this obviously holds iff both p, q are independent of θ_1, θ_2 . With regard to the definition of p, q , we have

$$\begin{aligned} s_{12} = 0, \quad s_{34} = 0, \quad s_{13}\overline{s_{23}} + s_{14}\overline{s_{24}} = 0, \quad \overline{s_{13}}s_{14} + \overline{s_{23}}s_{24} = 0, \\ s_{13}\overline{s_{24}} = 0, \quad s_{14}\overline{s_{23}} = 0. \end{aligned}$$

Hence $s_{12} = 0, s_{34} = 0$, and it is easy to see that at least three elements from the set $\{s_{13}, s_{14}, s_{23}, s_{24}\}$ have to vanish as well. \square

Corollary 8.5. *The sets $\mathcal{D}_1, \mathcal{D}_2$ are one-element sets iff the lattice decouples either into separate edges of the length a , or into identical copies of L-shaped pairs of edges.*

Proof. See the previous proposition. If all the off-diagonal elements of S vanish, the system decouples into separate edges and we return to the situation considered above. The second possibility is that just one of the numbers $s_{13}, s_{14}, s_{23}, s_{24}$ is nonzero, then the system is decoupled into L-shaped edge pairs. More precisely, $s_{13} \neq 0, s_{14} \neq 0, s_{23} \neq 0$ and $s_{24} \neq 0$ corresponds to $\lrcorner, \lrcorner, \lrcorner$ and \lrcorner shaped pairs, respectively, cf. Fig. 1 and the boundary conditions (6). \square

Apparently, if $s_{12} = s_{34} = 0$ and S contains just one nonzero off-diagonal element pair, the spectrum consists of isolated points.

8.3. Linearly growing spectral gaps, constant bands

Consider now the case when at least two off-diagonal elements of S are nonzero, i.e. the situation when both $\mathcal{D}_1, \mathcal{D}_2$ are intervals. Then the spectral asymptotics is determined by (25) where d is given by (28). Employing the symbols $\mathcal{D}_1, \mathcal{D}_2$ introduced

at the beginning of this section, we may characterize the values k corresponding to the spectrum as

$$k \in \bigcup_{j=1,2} \left(\frac{n\pi}{a} + \frac{d_j^\downarrow}{n\pi} + \mathcal{O}(n^{-2}), \frac{n\pi}{a} + \frac{d_j^\uparrow}{n\pi} + \mathcal{O}(n^{-2}) \right),$$

where $d_j^\downarrow = \min \mathcal{D}_j$, $d_j^\uparrow = \max \mathcal{D}_j$. Note that d_1^\pm, d_2^\pm depend only on S , since the term $(-1)^n$ can be absorbed into θ_1, θ_2 . The above relation gives spectral values in the form

$$k^2 \in \bigcup_{j=1,2} \left(\frac{n^2\pi^2}{a^2} + 2\frac{d_j^\downarrow}{a} + \mathcal{O}(n^{-1}), \frac{n^2\pi^2}{a^2} + 2\frac{d_j^\uparrow}{a} + \mathcal{O}(n^{-1}) \right), \quad (30)$$

which means that spectral bands (or their overlapping pairs) are of asymptotically constant width as the band number goes to infinity, and consequently, the spectral gaps are linearly growing with the band index. We also remark that the case a *nontrivial* δ'_s coupling considered in [Ex96, EG96] corresponds to S with all the entries nonzero and identical and thus has the described gap behaviour as expected.

The band structure depends on the parameter values, in particular, the band corresponding to \mathcal{D}_1 and \mathcal{D}_2 in (30) may or may not overlap. The former situation occurs, e.g., if only the elements s_{12} and s_{34} are nonzero, the latter if $s_{11} + s_{22} - s_{33} - s_{44}$ is large in comparison with the off-diagonal elements.

Let us finish this section with a short note on the prominent examples of the δ'_s and δ' coupling. A direct substitution of the appropriate boundary conditions into the expressions for d_j leads to these results:

- In the case of the δ'_s coupling, it holds $d_2^\uparrow = d_1^\downarrow = 0$. At the same time, one of the sets $\mathcal{D}_1, \mathcal{D}_2$ equals $\{d_2^\uparrow\}$. Consequently, the spectrum consists of asymptotically constant bands and linearly growing gaps between them. We remark that if $d_2^\uparrow = d_1^\downarrow$ and at the same time \mathcal{D}_1 and \mathcal{D}_2 are non-degenerate intervals, a special analysis is needed to find whether there is a gap between the bands corresponding to \mathcal{D}_1 and \mathcal{D}_2 or not.
- In the case of the δ' coupling, we have $d_2^\uparrow < d_1^\downarrow$, thus the sets \mathcal{D}_1 and \mathcal{D}_2 are disjoint. Consequently, the spectrum has asymptotically the pattern $\cdots GbgbGbgbGbgbG \cdots$ where G represents linearly growing gaps and b, g stand for bands and gaps whose widths are asymptotically constant.

Appendix: proof of Proposition 6.2

We will prove the claims in the order of their presentation:

(i) It holds $-K_c \cos^2 x + K_s \sin^2 x = \frac{-K_c + K_s}{2} - \frac{K_c + K_s}{2} \cos 2x$ and

$$\begin{aligned} & \max \{ \cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} \\ &= \max \{ \cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-2\pi, 0] \} \\ &= \max \{ \cos x \cdot L_c(\theta_1 - \pi, \theta_2 - \pi) + L(\theta_1 - \pi, \theta_2 - \pi) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} \\ &= \max \{ -\cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \}, \end{aligned}$$

therefore $V_2^+(x)$ equals

$$\frac{-K_c + K_s}{2} - \frac{K_c + K_s}{2} \cos 2x + \max \{ |\cos x| \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \},$$

and the function $V_2^+(x)$ can be treated in the same way. To finish the proof of (i), it suffices to realize that both $\cos 2x$ and $|\cos x|$ are π -periodic functions satisfying $\cos 2(\frac{\pi}{2} - x) = \cos 2x$ and $|\cos(\frac{\pi}{2} - x)| = |\cos x|$.

(ii) The part of $V_2^-(x)$ independent of θ_1, θ_2 is obviously increasing on $[0, \frac{\pi}{2}]$, because $-\cos 2x$ does. As for the second part, for all $x' \in [0, \frac{\pi}{2})$ it holds: if $\tilde{\theta}_1, \tilde{\theta}_2$ satisfy

$$\min \{ \cos x' \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} = \cos x' \cdot L_c(\tilde{\theta}_1, \tilde{\theta}_2) + L(\tilde{\theta}_1, \tilde{\theta}_2),$$

then $L_c(\tilde{\theta}_1, \tilde{\theta}_2) \leq 0$. If this was not the case one could shift both $\tilde{\theta}_1, \tilde{\theta}_2$ by π , which would change the sign of $L(\tilde{\theta}_1, \tilde{\theta}_2)$, and therefore make the value of $\cos x' \cdot L_c(\tilde{\theta}_1, \tilde{\theta}_2) + L(\tilde{\theta}_1, \tilde{\theta}_2)$ smaller, however, this would contradict the assumed minimality.

Let now $x'' < x' \in (0, \frac{\pi}{2}]$. Then $\cos x'' \cdot L_c(\tilde{\theta}_1, \tilde{\theta}_2) + L(\tilde{\theta}_1, \tilde{\theta}_2) \leq \cos x' \cdot L_c(\tilde{\theta}_1, \tilde{\theta}_2) + L(\tilde{\theta}_1, \tilde{\theta}_2)$, and therefore

$$\begin{aligned} \min \{ \cos x'' \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} \\ \leq \min \{ \cos x' \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \}, \end{aligned}$$

thus $\min \{ \cos x' \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \}$ is an increasing function of x in the interval $[0, \frac{\pi}{2}]$.

(iii) Let $\tilde{\theta}_1(x)$ and $\tilde{\theta}_2(x)$ be functions defined on $[0, \frac{\pi}{2}]$ such that

$$\begin{aligned} \max \{ \cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2) \mid \theta_1, \theta_2 \in (-\pi, \pi] \} \\ = \cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) + L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)); \end{aligned}$$

it follows that

$$\cos x \cdot \frac{\partial L_c}{\partial \tilde{\theta}_j}(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) + \frac{\partial L}{\partial \tilde{\theta}_j}(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) = 0, \quad j = 1, 2, \quad (31)$$

which we will use below. The function $V_2^+(x)$ can be then written as

$$V_2^+(x) = \frac{-K_c + K_s}{2} - \frac{K_c + K_s}{2} \cos 2x + \cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) + L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)),$$

so we can compute its derivative with respect to x ,

$$\begin{aligned} \frac{d}{dx} V_2^+(x) &= (K_c + K_s) \sin 2x - \sin x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) \\ &\quad + \cos x \left(\frac{\partial L_c}{\partial \tilde{\theta}_1} \tilde{\theta}_1'(x) + \frac{\partial L_c}{\partial \tilde{\theta}_2} \tilde{\theta}_2'(x) \right) + \frac{\partial L}{\partial \tilde{\theta}_1} \tilde{\theta}_1'(x) + \frac{\partial L}{\partial \tilde{\theta}_2} \tilde{\theta}_2'(x). \end{aligned}$$

The expression on the second line vanishes due to (31), hence

$$\frac{d}{dx} V_2^+(x) = \sin x \left[2(K_c + K_s) \cos x - L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) \right].$$

Now we will show that $\frac{d}{dx}V_2^+(x) \leq 0 \Rightarrow V_2^+(x) \geq 1$ — once this is proved, the proof of statement (iii) is finished. We have $\frac{d}{dx}V_2^+(x) \leq 0 \Rightarrow -K_c \cos x \geq K_s \cos x - \frac{1}{2}L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x))$. A substitution for $K_c \cos x$ into $V_2^+(x)$ gives the inequality

$$V_2^+(x) \geq K_s + \frac{1}{2} \cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) + L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)).$$

Since $K_s \geq 1$, it only remains to check that $\frac{1}{2} \cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) + L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) \geq 0$. The argument leans on the following two statements:

S1. $L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) \geq 0$.

S2. If $L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) < 0$, then $\cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) \geq 2|L(\tilde{\theta}_1(x), \tilde{\theta}_2(x))|$.

Statement *S1* can be demonstrated using the same idea as in part (ii) of this proof, *S2* can be proved by *reductio ad absurdum*. Let us suppose that $L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) < 0$ and $|\cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x))| < 2|L(\tilde{\theta}_1(x), \tilde{\theta}_2(x))|$. Then we define $\hat{\theta}_1 = \tilde{\theta}_1(x) + \rho$ and $\hat{\theta}_2 = \tilde{\theta}_2(x) + \rho$ where $\rho = \frac{\pi}{2}$ or $\rho = -\frac{\pi}{2}$ — the sign of ρ is chosen such that $L_c(\hat{\theta}_1, \hat{\theta}_2) \geq 0$. Then it holds

$$\begin{aligned} \cos x \cdot L_c(\hat{\theta}_1, \hat{\theta}_2) + L(\hat{\theta}_1, \hat{\theta}_2) &\geq \cos x \cdot 0 - L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) = |L(\tilde{\theta}_1(x), \tilde{\theta}_2(x))| \\ &> \frac{1}{2} \cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) > \frac{1}{2} \cos x \cdot L_c(\tilde{\theta}_1(x), \tilde{\theta}_2(x)) + L(\tilde{\theta}_1(x), \tilde{\theta}_2(x)), \end{aligned}$$

hence

$$V_2(x, \hat{\theta}_1, \hat{\theta}_2) > V_2(x, \tilde{\theta}_1(x), \tilde{\theta}_2(x)) = V_2^+(x),$$

which is in contradiction with the definition of $V_2^+(x)$.

(iv) It follows from their construction that the functions $V_2^+, V_2^-(x)$ satisfy $V_2^+(x) \geq V_2^-(x)$ for all $x \in (0, \frac{\pi}{2})$. The strict inequality $V_2^+(x) > V_2^-(x)$ is equivalent to the fact that the image of the function $\cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2)$ defined on $(-\pi, \pi]^2$ forms a non-degenerate interval. Since $\cos x \cdot L_c(\theta_1, \theta_2) + L(\theta_1, \theta_2)$ equals

$$\begin{aligned} \Re(-8 \cos ak(t_{11}\overline{t_{21}} + t_{12}\overline{t_{22}})e^{i\theta_1}) + \Re(8 \cos ak(t_{22}\overline{t_{21}} + \overline{t_{11}}t_{12})e^{i\theta_2}) \\ + \Re(8t_{11}\overline{t_{22}}e^{i(\theta_1-\theta_2)}) + \Re(8t_{12}\overline{t_{21}}e^{i(\theta_1+\theta_2)}) , \end{aligned}$$

i.e. it is of the type examined in Proposition 6.1, we infer that the image degenerates to a single point *iff*

$$t_{11}\overline{t_{21}} + t_{12}\overline{t_{22}} = 0 \quad \wedge \quad t_{22}\overline{t_{21}} + \overline{t_{11}}t_{12} = 0 \quad \wedge \quad t_{11}\overline{t_{22}} = 0 \quad \wedge \quad t_{12}\overline{t_{21}} = 0 ;$$

it is straightforward to check that these four conditions are satisfied *iff* at most one of the numbers $t_{11}, t_{12}, t_{21}, t_{22}$ is nonzero. This concludes the proof.

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